

# 3-ethoxy-2-butanone

Inchi:	InChI=1S/C6H12O2/c1-4-8-6(3)5(2)7/h6H,4H2,1-3H3
InchiKey:	UKIKCLGEESVZAE-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCOC(C)C(C)=O
Mol. weight [g/mol]:	116.16

## Physical Properties

Property code	Value	Unit	Source
gf	-236.72	kJ/mol	Joback Method
hf	-417.25	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	37.72	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	1.000		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpola	663.00		NIST Webbook
tb	412.53	K	Joback Method
tc	594.22	K	Joback Method
tf	214.54	K	Joback Method
vc	0.390	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.90	J/molxK	412.53	Joback Method
cpg	247.38	J/molxK	563.94	Joback Method
cpg	238.55	J/molxK	533.66	Joback Method
cpg	229.39	J/molxK	503.38	Joback Method
cpg	219.89	J/molxK	473.09	Joback Method
cpg	210.06	J/molxK	442.81	Joback Method
cpg	255.87	J/molxK	594.22	Joback Method
dvisc	0.0002624	Paxs	412.53	Joback Method
dvisc	0.0003438	Paxs	379.53	Joback Method

dvisc	0.0004742	Paxs	346.53	Joback Method
dvisc	0.0006998	Paxs	313.53	Joback Method
dvisc	0.0011317	Paxs	280.54	Joback Method
dvisc	0.0020807	Paxs	247.54	Joback Method
dvisc	0.0046134	Paxs	214.54	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R332680&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R332680&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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